



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:23 pm GMT

PDB ID : 4A82
Title : Fitted model of staphylococcus aureus sav1866 model ABC transporter in the human cystic fibrosis transmembrane conductance regulator volume map EMD-1966.
Authors : Rosenberg, M.F.; ORyan, L.P.; Hughes, G.; Zhao, Z.; Aleksandrov, L.A.; Riordan, J.R.; Ford, R.C.
Deposited on : 2011-11-18
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29102

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9248 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 CYSTIC FIBROSIS TRANSMEMBRANE CONDUCTANCE REGULATOR.

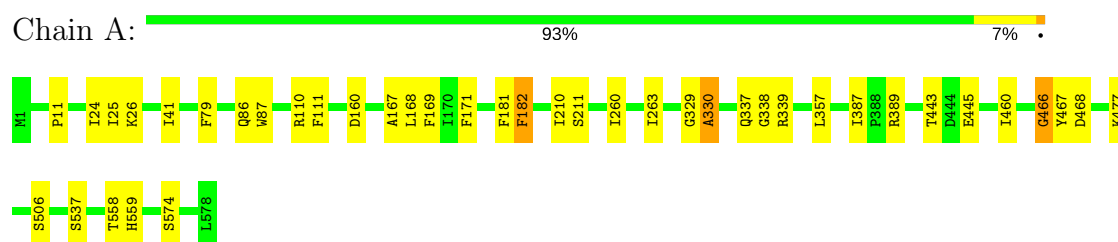
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	0	0	0
			2312	1156	578	578			
1	B	578	Total	C	N	O	0	0	0
			2312	1156	578	578			
1	C	578	Total	C	N	O	0	0	0
			2312	1156	578	578			
1	D	578	Total	C	N	O	0	0	0
			2312	1156	578	578			

3 Residue-property plots

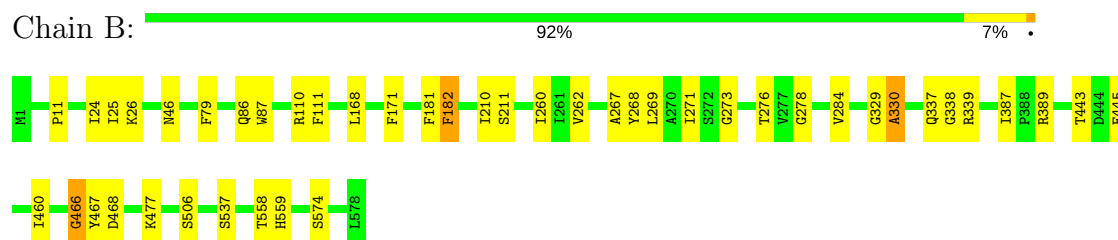
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

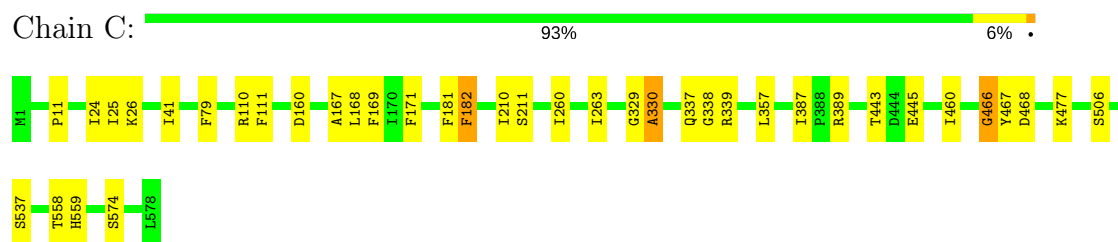
• Molecule 1: CYSTIC FIBROSIS TRANSMEMBRANE CONDUCTANCE REGULATOR



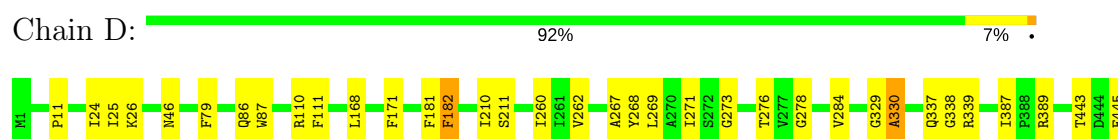
• Molecule 1: CYSTIC FIBROSIS TRANSMEMBRANE CONDUCTANCE REGULATOR



• Molecule 1: CYSTIC FIBROSIS TRANSMEMBRANE CONDUCTANCE REGULATOR



• Molecule 1: CYSTIC FIBROSIS TRANSMEMBRANE CONDUCTANCE REGULATOR





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.30 Å 75.80 Å 300.00 Å 90.00° 90.00° 125.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	60.8 (5.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	2DX	Depositor
R, R_{free}	0.370 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9248	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/2311	0.69	1/2887 (0.0%)
1	B	0.42	1/2311 (0.0%)	0.71	1/2887 (0.0%)
1	C	0.35	0/2311	0.69	1/2887 (0.0%)
1	D	0.42	1/2311 (0.0%)	0.71	1/2887 (0.0%)
All	All	0.38	2/9244 (0.0%)	0.70	4/11548 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	ASN	C-N	-9.48	1.12	1.34
1	D	46	ASN	C-N	-9.46	1.12	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	357	LEU	N-CA-C	-5.17	97.03	111.00
1	A	357	LEU	N-CA-C	-5.17	97.03	111.00
1	B	46	ASN	O-C-N	5.11	130.87	122.70
1	D	46	ASN	O-C-N	5.08	130.83	122.70

There are no chirality outliers.

There are no planarity outliers.

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	2312	0	639	20	0
1	B	2312	0	638	23	0
1	C	2312	0	639	19	0
1	D	2312	0	638	24	0
All	All	9248	0	2554	86	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 7.

All (86) 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:B:387:ILE:C	1:B:389:ARG:H	1.99	0.66
1:D:387:ILE:C	1:D:389:ARG:H	1.99	0.66
1:A:387:ILE:C	1:A:389:ARG:H	1.99	0.64
1:C:387:ILE:C	1:C:389:ARG:H	1.99	0.64
1:C:167:ALA:O	1:C:169:PHE:N	2.36	0.59
1:A:167:ALA:O	1:A:169:PHE:N	2.36	0.59
1:D:24:ILE:C	1:D:26:LYS:H	2.07	0.58
1:B:24:ILE:C	1:B:26:LYS:H	2.07	0.57
1:C:24:ILE:C	1:C:26:LYS:H	2.07	0.57
1:A:24:ILE:C	1:A:26:LYS:H	2.07	0.57
1:A:210:ILE:O	1:A:211:SER:C	2.45	0.56
1:D:387:ILE:C	1:D:389:ARG:N	2.59	0.56
1:C:210:ILE:O	1:C:211:SER:C	2.45	0.55
1:A:387:ILE:C	1:A:389:ARG:N	2.60	0.55
1:D:276:THR:C	1:D:278:GLY:H	2.09	0.55
1:A:24:ILE:O	1:A:26:LYS:N	2.40	0.54
1:B:276:THR:C	1:B:278:GLY:H	2.09	0.54
1:C:387:ILE:C	1:C:389:ARG:N	2.60	0.54
1:C:466:GLY:O	1:C:468:ASP:N	2.41	0.54
1:B:387:ILE:C	1:B:389:ARG:N	2.59	0.54
1:D:210:ILE:O	1:D:211:SER:C	2.46	0.54
1:A:466:GLY:O	1:A:468:ASP:N	2.41	0.54
1:D:24:ILE:O	1:D:26:LYS:N	2.42	0.53
1:B:210:ILE:O	1:B:211:SER:C	2.46	0.53
1:B:466:GLY:O	1:B:468:ASP:N	2.42	0.53
1:B:181:PHE:O	1:B:182:PHE:C	2.48	0.53
1:A:181:PHE:O	1:A:182:PHE:C	2.47	0.52
1:B:24:ILE:O	1:B:26:LYS:N	2.42	0.52
1:D:466:GLY:O	1:D:468:ASP:N	2.42	0.52
1:C:24:ILE:O	1:C:26:LYS:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:PHE:O	1:C:182:PHE:C	2.47	0.52
1:B:267:ALA:C	1:B:269:LEU:H	2.13	0.52
1:D:267:ALA:C	1:D:269:LEU:H	2.13	0.52
1:D:337:GLN:O	1:D:339:ARG:N	2.43	0.52
1:C:337:GLN:O	1:C:339:ARG:N	2.43	0.51
1:B:337:GLN:O	1:B:339:ARG:N	2.43	0.51
1:D:181:PHE:O	1:D:182:PHE:C	2.48	0.51
1:A:337:GLN:O	1:A:339:ARG:N	2.43	0.51
1:C:443:THR:C	1:C:445:GLU:N	2.66	0.49
1:A:443:THR:C	1:A:445:GLU:N	2.66	0.48
1:D:110:ARG:O	1:D:111:PHE:C	2.52	0.48
1:C:110:ARG:O	1:C:111:PHE:C	2.53	0.47
1:A:460:ILE:O	1:A:466:GLY:HA2	2.15	0.47
1:B:443:THR:C	1:B:445:GLU:N	2.67	0.47
1:B:110:ARG:O	1:B:111:PHE:C	2.52	0.46
1:C:167:ALA:C	1:C:169:PHE:H	2.19	0.46
1:A:558:THR:O	1:A:559:HIS:C	2.54	0.46
1:D:443:THR:C	1:D:445:GLU:N	2.67	0.46
1:D:460:ILE:O	1:D:466:GLY:HA2	2.16	0.46
1:B:558:THR:O	1:B:559:HIS:C	2.54	0.46
1:A:110:ARG:O	1:A:111:PHE:C	2.53	0.46
1:C:460:ILE:O	1:C:466:GLY:HA2	2.15	0.46
1:B:276:THR:C	1:B:278:GLY:N	2.70	0.45
1:A:167:ALA:C	1:A:169:PHE:H	2.19	0.45
1:B:460:ILE:O	1:B:466:GLY:HA2	2.16	0.45
1:D:558:THR:O	1:D:559:HIS:C	2.54	0.45
1:C:558:THR:O	1:C:559:HIS:C	2.54	0.45
1:A:167:ALA:C	1:A:169:PHE:N	2.70	0.45
1:D:260:ILE:C	1:D:262:VAL:H	2.20	0.45
1:B:260:ILE:C	1:B:262:VAL:H	2.21	0.45
1:D:260:ILE:C	1:D:262:VAL:N	2.70	0.45
1:D:276:THR:C	1:D:278:GLY:N	2.70	0.44
1:C:260:ILE:O	1:C:263:ILE:N	2.50	0.44
1:A:260:ILE:O	1:A:263:ILE:N	2.50	0.44
1:C:167:ALA:C	1:C:169:PHE:N	2.70	0.44
1:C:329:GLY:O	1:C:330:ALA:C	2.56	0.43
1:A:466:GLY:C	1:A:468:ASP:N	2.72	0.43
1:D:329:GLY:O	1:D:330:ALA:C	2.57	0.43
1:A:329:GLY:O	1:A:330:ALA:C	2.56	0.43
1:B:260:ILE:C	1:B:262:VAL:N	2.70	0.43
1:D:466:GLY:C	1:D:468:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLY:O	1:B:330:ALA:C	2.57	0.43
1:C:24:ILE:C	1:C:26:LYS:N	2.72	0.42
1:B:260:ILE:O	1:B:262:VAL:N	2.52	0.42
1:D:24:ILE:C	1:D:26:LYS:N	2.73	0.42
1:B:466:GLY:C	1:B:468:ASP:N	2.72	0.42
1:C:466:GLY:C	1:C:468:ASP:N	2.72	0.42
1:A:24:ILE:C	1:A:26:LYS:N	2.72	0.42
1:D:271:ILE:C	1:D:273:GLY:H	2.22	0.42
1:B:24:ILE:C	1:B:26:LYS:N	2.73	0.42
1:B:271:ILE:C	1:B:273:GLY:H	2.22	0.42
1:D:260:ILE:O	1:D:262:VAL:N	2.52	0.42
1:B:86:GLN:O	1:B:87:TRP:C	2.58	0.41
1:A:86:GLN:O	1:A:87:TRP:C	2.58	0.41
1:D:86:GLN:O	1:D:87:TRP:C	2.57	0.41
1:D:267:ALA:C	1:D:269:LEU:N	2.74	0.40

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	576/578 (100%)	485 (84%)	75 (13%)	16 (3%)	6	2
1	B	576/578 (100%)	479 (83%)	81 (14%)	16 (3%)	6	2
1	C	576/578 (100%)	485 (84%)	75 (13%)	16 (3%)	6	2
1	D	576/578 (100%)	480 (83%)	80 (14%)	16 (3%)	6	2
All	All	2304/2312 (100%)	1929 (84%)	311 (14%)	64 (3%)	6	2

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	41	ILE
1	A	338	GLY
1	B	25	ILE
1	B	338	GLY
1	C	25	ILE
1	C	41	ILE
1	C	338	GLY
1	D	25	ILE
1	D	338	GLY
1	A	160	ASP
1	A	168	LEU
1	A	182	PHE
1	A	466	GLY
1	A	467	TYR
1	A	506	SER
1	B	182	PHE
1	B	466	GLY
1	B	467	TYR
1	B	506	SER
1	C	160	ASP
1	C	168	LEU
1	C	182	PHE
1	C	466	GLY
1	C	467	TYR
1	C	506	SER
1	D	182	PHE
1	D	466	GLY
1	D	467	TYR
1	D	506	SER
1	A	79	PHE
1	A	330	ALA
1	A	574	SER
1	B	79	PHE
1	B	330	ALA
1	B	477	LYS
1	B	574	SER
1	C	79	PHE
1	C	330	ALA
1	C	574	SER
1	D	79	PHE
1	D	330	ALA
1	D	477	LYS

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Mol	Chain	Res	Type
1	D	574	SER
1	A	477	LYS
1	A	537	SER
1	B	168	LEU
1	B	268	TYR
1	B	537	SER
1	C	477	LYS
1	C	537	SER
1	D	168	LEU
1	D	268	TYR
1	D	537	SER
1	D	11	PRO
1	A	11	PRO
1	B	11	PRO
1	C	11	PRO
1	B	171	PHE
1	B	284	VAL
1	D	171	PHE
1	D	284	VAL
1	A	171	PHE
1	C	171	PHE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 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.