



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4ORA
Title : Crystal structure of a human calcineurin mutant
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Deposited on : 2014-02-11
Resolution : 2.75 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

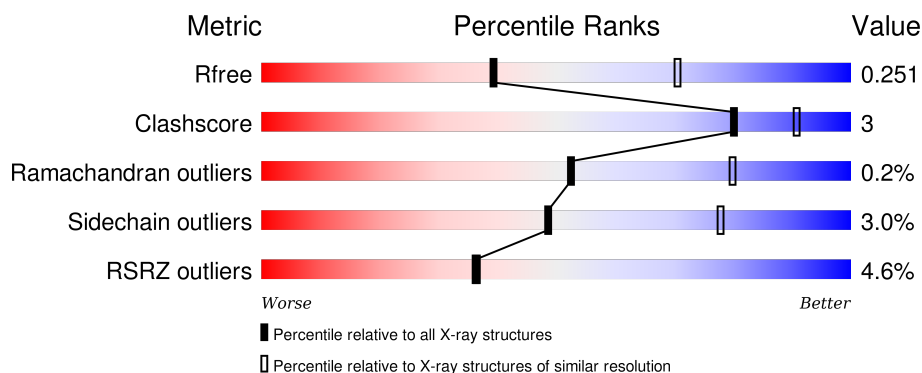
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
R_{free}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	544	<div> <div>5%</div> <div>63%</div> <div>9%</div> <div>27%</div> </div>
2	B	170	<div> <div>%</div> <div>90%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	601	-	-	-	X
4	FE	A	602	-	-	-	X
5	CA	B	202	-	-	-	X
5	CA	B	203	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4614 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 Serine/threonine-protein phosphatase 2B catalytic subunit beta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	3	0
			3239	2085	543	591	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P16298
A	-18	GLY	-	EXPRESSION TAG	UNP P16298
A	-17	SER	-	EXPRESSION TAG	UNP P16298
A	-16	SER	-	EXPRESSION TAG	UNP P16298
A	-15	HIS	-	EXPRESSION TAG	UNP P16298
A	-14	HIS	-	EXPRESSION TAG	UNP P16298
A	-13	HIS	-	EXPRESSION TAG	UNP P16298
A	-12	HIS	-	EXPRESSION TAG	UNP P16298
A	-11	HIS	-	EXPRESSION TAG	UNP P16298
A	-10	HIS	-	EXPRESSION TAG	UNP P16298
A	-9	SER	-	EXPRESSION TAG	UNP P16298
A	-8	SER	-	EXPRESSION TAG	UNP P16298
A	-7	GLY	-	EXPRESSION TAG	UNP P16298
A	-6	LEU	-	EXPRESSION TAG	UNP P16298
A	-5	VAL	-	EXPRESSION TAG	UNP P16298
A	-4	PRO	-	EXPRESSION TAG	UNP P16298
A	-3	ARG	-	EXPRESSION TAG	UNP P16298
A	-2	GLY	-	EXPRESSION TAG	UNP P16298
A	-1	SER	-	EXPRESSION TAG	UNP P16298
A	0	HIS	-	EXPRESSION TAG	UNP P16298
A	418	TYR	VAL	ENGINEERED MUTATION	UNP P16298
A	419	LEU	PHE	ENGINEERED MUTATION	UNP P16298

- Molecule 2 is a protein called Calcineurin subunit B type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1324	836	219	261	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	Ca	0	0
			4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		
6	B	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.20Å 108.20Å 284.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.99 – 2.75 46.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (46.99-2.75) 92.0 (46.99-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.20 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.199 , 0.249 0.204 , 0.251	Depositor DCC
R_{free} test set	1247 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24488 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3338	0.61	0/4532
2	B	0.52	0/1343	0.60	0/1797
All	All	0.49	0/4681	0.61	0/6329

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3239	0	3160	26	0
2	B	1324	0	1304	8	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	B	4	0	0	0	0
6	A	34	0	0	0	0
6	B	11	0	0	0	0
All	All	4614	0	4464	31	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 3.

All (31) 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:360:THR:HG23	2:B:159:LEU:HD21	1.84	0.60
1:A:255:GLU:O	1:A:270:ASN:ND2	2.34	0.60
1:A:167[B]:GLU:HG3	1:A:172:LYS:HD2	1.85	0.57
2:B:51:ASN:HB3	2:B:54:VAL:HG23	1.87	0.55
1:A:278:LEU:HD21	1:A:286:ILE:HG13	1.89	0.55
2:B:100:MET:HG3	2:B:110:GLU:HG2	1.88	0.55
2:B:61:PHE:O	2:B:73:GLU:HB3	2.09	0.53
1:A:77:GLY:HA3	1:A:143:TRP:CD1	2.44	0.53
1:A:384:ASP:N	1:A:384:ASP:OD1	2.43	0.52
1:A:114:GLY:O	1:A:332:LYS:NZ	2.46	0.48
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.73	0.47
1:A:288:ARG:NH2	1:A:291:GLU:OE1	2.49	0.46
1:A:66:ASP:HB2	1:A:69:ILE:HD12	1.97	0.46
1:A:149:TYR:HB3	1:A:152:THR:OG1	2.16	0.46
1:A:338:MET:HE3	1:A:338:MET:HB3	1.90	0.45
1:A:372:GLU:O	1:A:376:ASN:ND2	2.47	0.45
1:A:225:ASP:O	1:A:228:LYS:HE3	2.18	0.44
1:A:93:PRO:CB	1:A:334:GLU:HG2	2.47	0.44
1:A:357:ASP:OD2	1:A:359:PHE:HB2	2.17	0.44
1:A:20:PRO:HA	1:A:21:PRO:HD3	1.94	0.43
1:A:377:VAL:HG13	2:B:29:LEU:HD11	2.00	0.43
1:A:358:VAL:HB	2:B:115:LEU:HD21	2.01	0.43
1:A:210:GLY:HA3	1:A:269:TYR:CE2	2.55	0.42
1:A:363:LEU:HB3	1:A:364:PRO:HD3	2.00	0.42
1:A:38:LEU:HG	1:A:58:HIS:CD2	2.54	0.42
2:B:111:LEU:HD12	2:B:111:LEU:HA	1.84	0.41
2:B:160:ASP:HA	2:B:162:HIS:CE1	2.56	0.41
1:A:99:ASP:N	1:A:99:ASP:OD1	2.53	0.40
1:A:302:LYS:HD3	1:A:307:GLY:O	2.21	0.40
1:A:418:TYR:HA	1:A:418:TYR:HD1	1.74	0.40
1:A:383:ASP:C	1:A:385:GLU:H	2.25	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	394/544 (72%)	376 (95%)	17 (4%)	1 (0%)	46	74
2	B	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
All	All	558/714 (78%)	538 (96%)	19 (3%)	1 (0%)	52	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ARG

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	359/470 (76%)	345 (96%)	14 (4%)	39	69
2	B	148/151 (98%)	147 (99%)	1 (1%)	88	96
All	All	507/621 (82%)	492 (97%)	15 (3%)	48	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	83	ARG
1	A	85	LYS
1	A	99	ASP
1	A	112	GLU

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Mol	Chain	Res	Type
1	A	153	LEU
1	A	177	ILE
1	A	217	THR
1	A	288	ARG
1	A	383	ASP
1	A	384	ASP
1	A	417	ARG
1	A	418	TYR
1	A	480	GLU
2	B	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	80	GLN
2	B	89	GLN

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 [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - 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.

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 ⓘ

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, 95th 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	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/544 (72%)	-0.19	25 (6%) 23 23	14, 29, 97, 132	0
2	B	166/170 (97%)	-0.20	1 (0%) 90 92	23, 38, 65, 83	0
All	All	563/714 (78%)	-0.19	26 (4%) 36 36	14, 32, 80, 132	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	6.1
1	A	386	LEU	5.6
2	B	4	ALA	5.3
1	A	416	ALA	5.0
1	A	481	GLU	4.6
1	A	484	GLY	4.5
1	A	487	ARG	4.5
1	A	421	VAL	3.8
1	A	478	SER	3.7
1	A	479	PHE	3.6
1	A	485	LEU	3.6
1	A	488	ILE	3.4
1	A	422	LEU	3.2
1	A	494	PRO	3.2
1	A	252	LYS	3.1
1	A	482	ALA	2.9
1	A	491	ARG	2.7
1	A	259	HIS	2.7
1	A	486	ASP	2.5
1	A	480	GLU	2.5
1	A	254	GLN	2.4
1	A	382	SER	2.4
1	A	384	ASP	2.3
1	A	417	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	ASN	2.1
1	A	420	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
4	FE	A	602	1/1	0.94	0.65	7.65	23,23,23,23	0
3	ZN	A	601	1/1	0.95	0.62	7.57	23,23,23,23	0
5	CA	B	203	1/1	0.93	0.26	5.60	32,32,32,32	0
5	CA	B	202	1/1	0.90	0.26	3.95	42,42,42,42	0
5	CA	B	204	1/1	0.92	0.21	1.09	42,42,42,42	0
5	CA	B	201	1/1	0.88	0.14	-0.96	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.