



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6BBI / pdb_00006bbi
Title : The CRAC channel Orai in an unlatched-closed conformation; K163W loss-of-function mutation; P42212 crystal form
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Deposited on : 2017-10-18
Resolution : 4.35 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

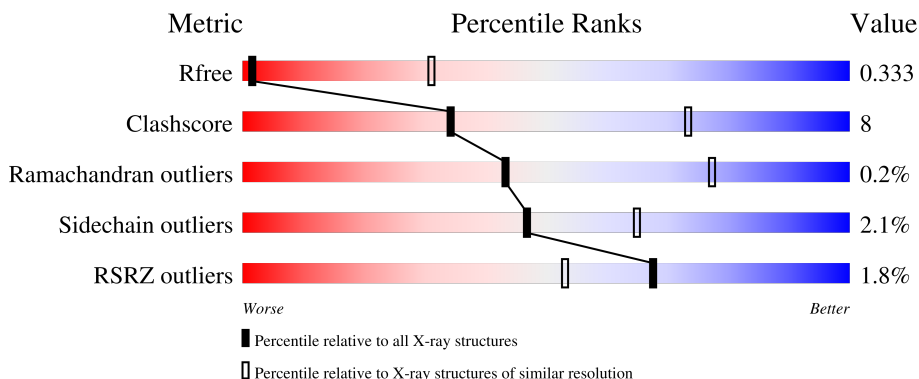
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.35 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}	180053	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	214	
1	B	214	
1	C	214	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3338 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 Calcium release-activated calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1151	768	180	192	11	0	0	0
1	B	138	1036	698	161	168	9	0	0	0
1	C	152	1151	768	180	192	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	TRP	LYS	engineered mutation	UNP Q9U6B8
A	224	SER	CYS	engineered mutation	UNP Q9U6B8
A	283	THR	CYS	engineered mutation	UNP Q9U6B8
A	342	GLU	-	expression tag	UNP Q9U6B8
A	343	GLY	-	expression tag	UNP Q9U6B8
A	344	GLU	-	expression tag	UNP Q9U6B8
A	345	GLU	-	expression tag	UNP Q9U6B8
A	346	PHE	-	expression tag	UNP Q9U6B8
B	163	TRP	LYS	engineered mutation	UNP Q9U6B8
B	224	SER	CYS	engineered mutation	UNP Q9U6B8
B	283	THR	CYS	engineered mutation	UNP Q9U6B8
B	342	GLU	-	expression tag	UNP Q9U6B8
B	343	GLY	-	expression tag	UNP Q9U6B8
B	344	GLU	-	expression tag	UNP Q9U6B8
B	345	GLU	-	expression tag	UNP Q9U6B8
B	346	PHE	-	expression tag	UNP Q9U6B8
C	163	TRP	LYS	engineered mutation	UNP Q9U6B8
C	224	SER	CYS	engineered mutation	UNP Q9U6B8
C	283	THR	CYS	engineered mutation	UNP Q9U6B8
C	342	GLU	-	expression tag	UNP Q9U6B8
C	343	GLY	-	expression tag	UNP Q9U6B8
C	344	GLU	-	expression tag	UNP Q9U6B8
C	345	GLU	-	expression tag	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	PHE	-	expression tag	UNP Q9U6B8

4 Data and refinement statistics i

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.70Å 118.70Å 122.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 4.35 19.85 – 4.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.85-4.35) 98.4 (19.85-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 4.36Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.306 , 0.329 0.309 , 0.333	Depositor DCC
R_{free} test set	592 reflections (9.78%)	wwPDB-VP
Wilson B-factor (Å ²)	272.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 274.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k 0.014 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3338	wwPDB-VP
Average B, all atoms (Å ²)	329.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.36	0/1180	0.80	3/1607 (0.2%)
1	B	0.42	1/1065 (0.1%)	0.83	4/1456 (0.3%)
1	C	0.39	1/1180 (0.1%)	0.86	5/1607 (0.3%)
All	All	0.39	2/3425 (0.1%)	0.83	12/4670 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	287	ILE	C-N	6.28	1.42	1.33
1	B	259	PHE	C-N	5.93	1.41	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	ILE	CA-C-N	8.47	128.05	119.24
1	C	287	ILE	C-N-CA	8.47	128.05	119.24
1	C	276	PRO	N-CA-C	5.98	117.99	110.70
1	A	276	PRO	N-CA-C	5.96	117.97	110.70
1	B	276	PRO	N-CA-C	5.96	117.97	110.70

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	1151	0	1151	20	0
1	B	1036	0	1034	23	0
1	C	1151	0	1151	22	0
All	All	3338	0	3336	51	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 8.

The worst 5 of 51 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:155:ARG:HD2	1:B:152:GLN:HE22	1.66	0.60
1:C:312:THR:O	1:C:316:ILE:HG12	2.03	0.59
1:B:276:PRO:HB2	1:B:277:PRO:HD3	1.88	0.56
1:C:276:PRO:HB2	1:C:277:PRO:HD3	1.87	0.55
1:A:276:PRO:HB2	1:A:277:PRO:HD3	1.92	0.52

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	146/214 (68%)	139 (95%)	7 (5%)	0	100	100
1	B	132/214 (62%)	126 (96%)	6 (4%)	0	100	100
1	C	146/214 (68%)	140 (96%)	5 (3%)	1 (1%)	18	55
All	All	424/642 (66%)	405 (96%)	18 (4%)	1 (0%)	43	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	TYR

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	117/190 (62%)	114 (97%)	3 (3%)	40	60
1	B	104/190 (55%)	102 (98%)	2 (2%)	50	66
1	C	117/190 (62%)	115 (98%)	2 (2%)	53	67
All	All	338/570 (59%)	331 (98%)	7 (2%)	47	65

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	MET
1	B	287	ILE
1	C	287	ILE
1	C	207	MET
1	A	287	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	307	HIS
1	C	152	GLN
1	C	307	HIS
1	A	307	HIS
1	A	206	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 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, 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	152/214 (71%)	-0.24	1 (0%) 84 71	206, 320, 428, 488	0
1	B	138/214 (64%)	-0.20	3 (2%) 62 48	170, 313, 480, 559	0
1	C	152/214 (71%)	-0.01	4 (2%) 57 44	197, 309, 446, 537	0
All	All	442/642 (68%)	-0.15	8 (1%) 67 53	170, 314, 455, 559	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	3.9
1	C	214	THR	3.0
1	C	159	LYS	2.4
1	C	260	LEU	2.2
1	A	296	PHE	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.