wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 02:24 PM EDT

PDB ID	:	6BBI
Title	:	The CRAC channel Orai in an unlatched-closed conformation; K163W loss-of-function mutation; P42212 crystal form
Authors	:	Long, S.B.; Hou, X.; Burstein, S.
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 (i) 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 (1)) were used in the production of this report:

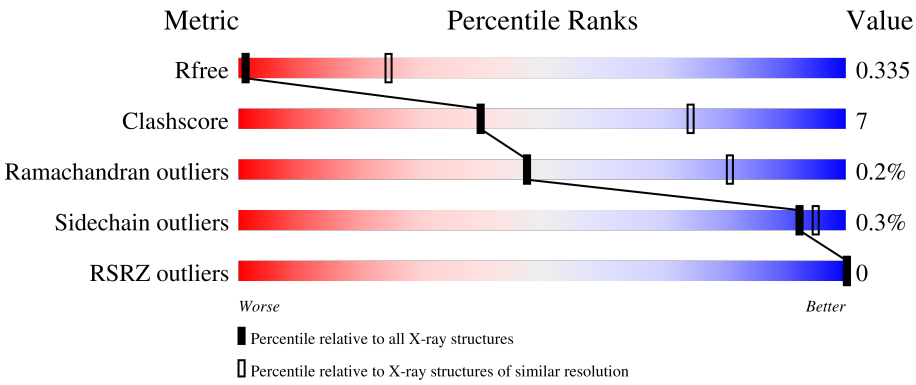
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)
RSRZ outliers	127900	1078 (4.92-3.70)

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 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 <=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	60% 11% 29%
1	B	214	53% 11% 36%
1	C	214	57% 14% 29%

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: Calcium release-activated calcium channel protein 1

Chain A: 60% 11% 29%

MET SER GLN SER GLY GLU ASP LEU HIS SER PRO THR TYR LEU SER W148 R155 W163 A166 L167 M176 V179 Q180 LEU ASP HIS ASP THR ASN VAL PRO P189 I193 A196 A204 C215 N219 ILE GLU THR VAL SER ASN LEU HIS SER ILE SER LEU VAL

HIS GLU SER PRO HIS GLU ARG L240 F250 L253 L254 G255 L256 I263 A264 P276 P277 A282 V285 M290 M294 I298 E327 GLN ASP HIS LEU GLU HIS HIS ASN ASN ILE ARG ASN ASN GLY GLU GLY GLU GLU PHE

• Molecule 1: Calcium release-activated calcium channel protein 1

Chain B: 53% 11% 36%

MET SER GLN SER GLY GLU ASP LEU HIS SER PRO THR TYR LEU SER W148 Q152 W163 T164 V174 A175 M176 V177 E178 V179 Q180 LEU ASP HIS ASP THR ASN VAL PRO P189 I193 A204 C215 N219 ILE GLU THR VAL SER ASN LEU HIS SER ILE SER LEU VAL HIS

GLU SER PRO HIS GLU ARG L240 L253 L256 L260 I263 A264 P276 P277 A278 A282 V285 M290 M294 I298 H299 F300 V313 SER GLY ILE ARG GLU LEU GLU MET LEU LYS GLU GLN MET GLU GLN ASP HIS LEU GLU HIS HIS ASN ASN ILE ARG ASN

ASN GLY GLU GLY GLU GLU PHE

• Molecule 1: Calcium release-activated calcium channel protein 1

Chain C: 57% 14% 29%

MET SER GLN SER GLY GLU ASP LEU HIS SER PRO THR TYR LEU SER W148 W163 L167 V174 A175 M176 V177 E178 V179 Q180 LEU ASP HIS ASP THR ASN VAL PRO P189 N219 ILE GLU THR VAL SER ASN LEU HIS SER ILE SER LEU VAL HIS GLU SER PRO HIS GLU ARG L240

L253 L256 I257 L260 I263 A264 I265 L266 Y272 P276 P277 A278 A282 V285 L286 I287 P288 V289 M290 F293 M294 I298 H299 F300 T312 I316 R317 E318 L319 E320 K321 L322 E327 GLN ASP HIS LEU GLU GLU HIS HIS ASN ASN ILE ARG ASN ASN GLY

GLU GLY GLU GLU PHE

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) 99.8 (19.85-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 4.36Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.306 , 0.329 0.305 , 0.335	Depositor DCC
R_{free} test set	592 reflections (9.80%)	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)	0.20 , 220.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/1180	0.47	0/1607
1	B	0.32	0/1065	0.50	0/1456
1	C	0.31	0/1180	0.49	0/1607
All	All	0.32	0/3425	0.49	0/4670

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 (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	18	0
1	B	1036	0	1034	23	0
1	C	1151	0	1151	22	0
All	All	3338	0	3336	49	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.

The worst 5 of 49 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	22	62
All	All	424/642 (66%)	405 (96%)	18 (4%)	1 (0%)	47	81

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%)	117 (100%)	0	100	100
1	B	104/190 (55%)	104 (100%)	0	100	100
1	C	117/190 (62%)	116 (99%)	1 (1%)	78	88
All	All	338/570 (59%)	337 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	TRP

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

Mol	Chain	Res	Type
1	A	206	HIS
1	B	152	GLN
1	C	152	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 monosaccharides 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%)	-0.65	0	100	100	206, 320, 428, 488	0
1	B	138/214 (64%)	-0.58	0	100	100	170, 313, 480, 559	0
1	C	152/214 (71%)	-0.53	0	100	100	197, 309, 446, 537	0
All	All	442/642 (68%)	-0.59	0	100	100	170, 314, 455, 559	0

There are no RSRZ outliers to report.

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 monosaccharides 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.